Force field optimization: To provide a training set of QM data to train ReaxFF for NaClO4, we use the B3LYP hybrid flavour of the density functional method with the 6-311+G(d,p) basis set. All QM calculations were conducted using Jaguar 8.8. During the force field optimization procedure, the cost objective function was expressed as deviations between QM and ReaxFF energies and forces as in Eq. (1). Here, x_(i,QM) and x_(i,ReaxFF) are the corresponding values for the QM and ReaxFF results, respectively, and σ_i is the weight parameter adjusted based on the accuracy in the training data.

$$Error = \sum_{i=1}^{n} \left[\frac{\left(x_{i,QM} - x_{i,\mathrm{Re}\,axFF}\right)}{\sigma_i} \right]^2 \qquad \text{Eq. (1)}$$

The detailed formation mechanisms of major products

- **NaF formation**: NaF is formed by the defluorination reaction from FEC via Path 1, as shown in **Figure 2** and **Figure S7a-c**;
- **NaOH formation**: NaOH comes from the hydration of Na_2O_2 and Na_2O, especially when excessive Na^0 is present, as shown in **Figure 4** and **Figure S2**.
- **Na_2CO_3 formation**: CO_3^{2-} is formed by the reduction of PC and FEC via path 2 and path 3, as shown in **Figure 2, Figure 3** and **Figure S7d-f**;
- **Na_2O and Na_2O_2 formation**: The reduction of PC and FEC supplied a large amount of oxygen atoms, leading to the formation of Na_2O_2 and Na_2O, as shown in **Figure S7h**.
- **C_3H_6 formation**: C_3H_6 is from the reduction of PC to release CO_3^{2-} via Path 3, as shown in **Figure 2** and **Figure S7j-l**;
- **NaCl and $NaClO_x$ formation**: ClO_4^- anions sequentially reduce into ClO_x^-(x=3,2,1) accompanied by O_2^- release (**Figure S7g-h)**, eventually forming Cl^-;

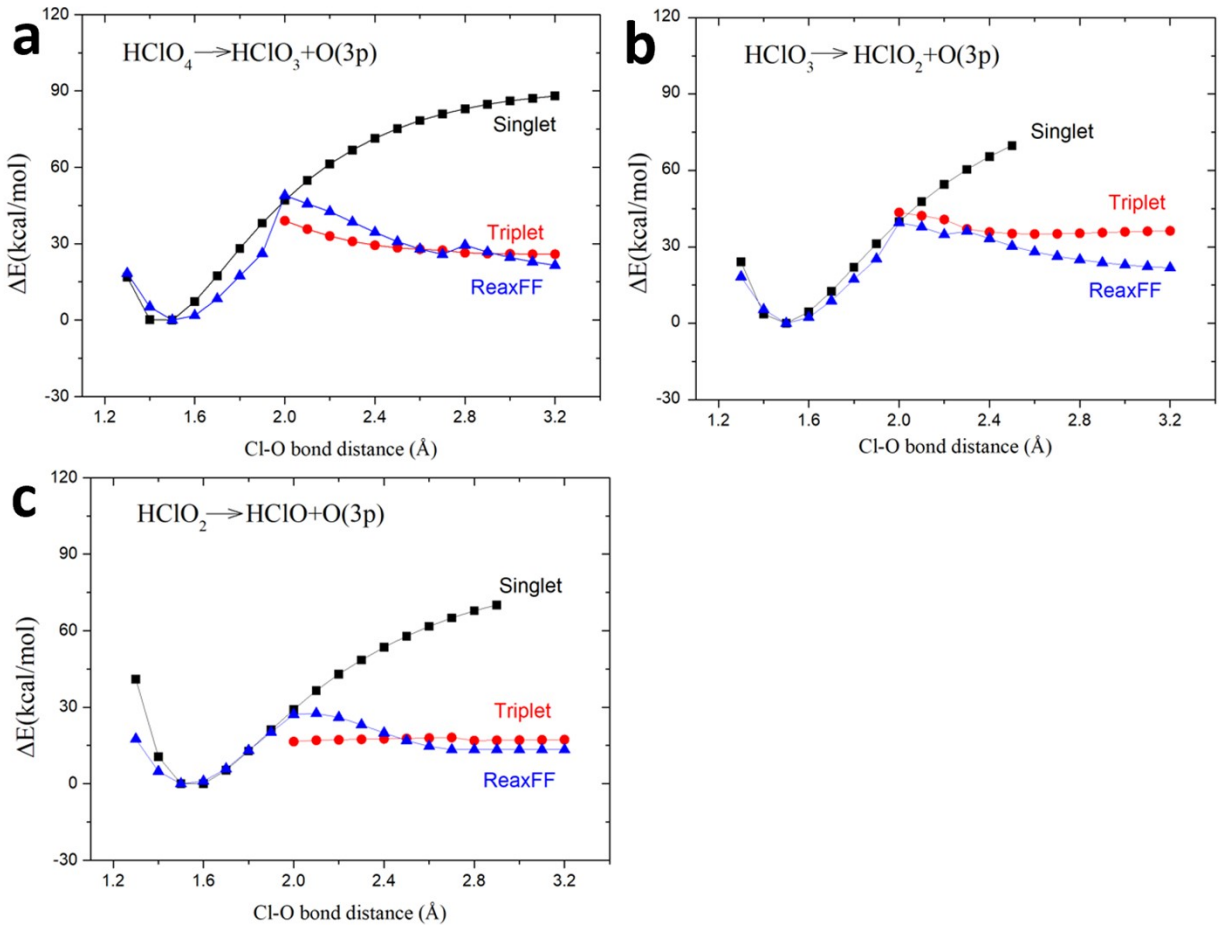

Figure S1. Cl-O bond dissociation curves for the QM and ReaxFF results. (a) The Cl-O bond dissociation curves for $HClO_4$. (b) The Cl-O bond dissociation curves for $HClO_3$. (c) The Cl-O bond dissociation curves for $HClO_2$.

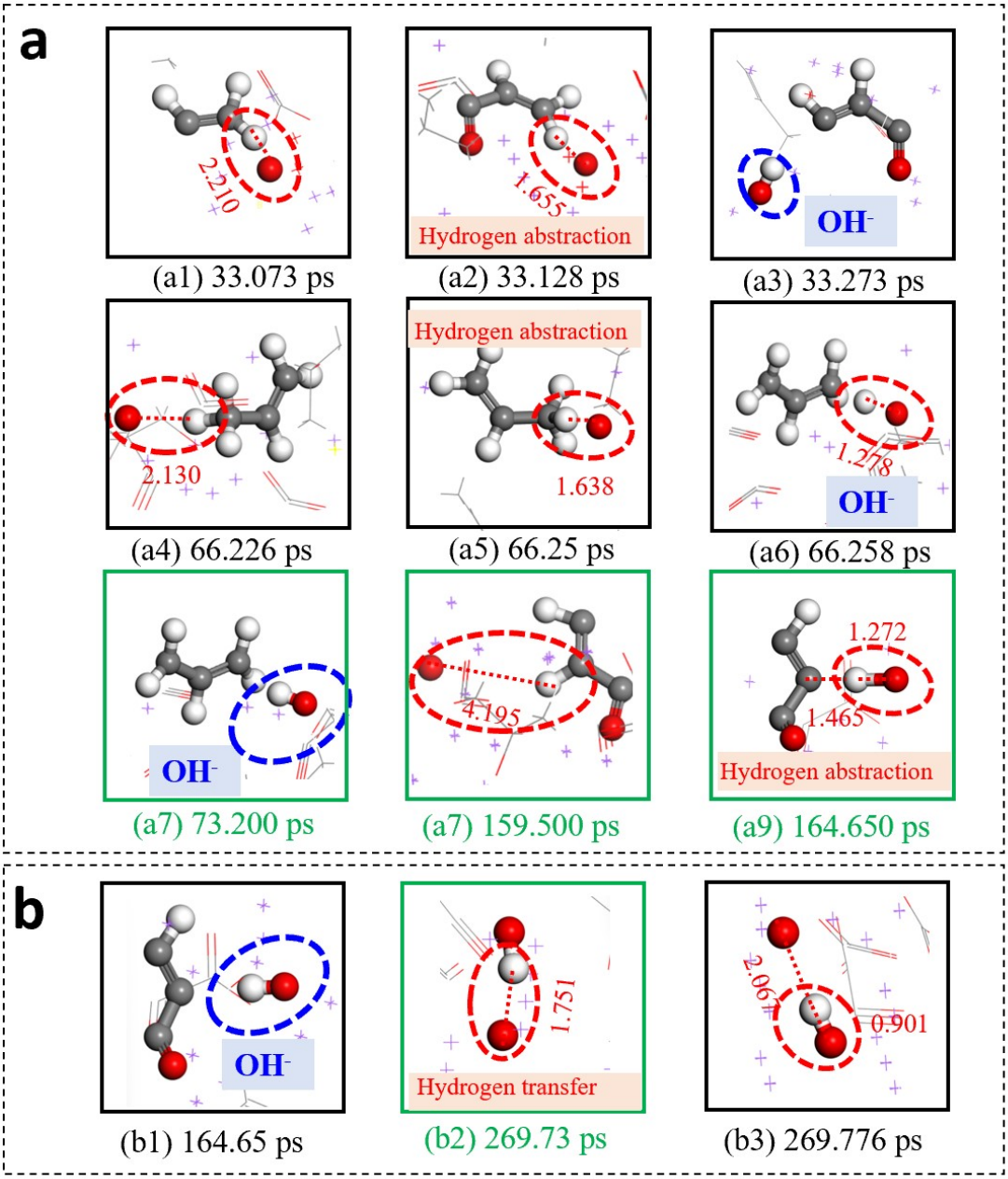

Figure S2. Sequence for OH^- formation obtained from HAIR simulations between 33.073 ps and 269.776 ps. (a) OH^- formation via a hydrogen abstraction process. (b) OH^- formation via a hydrogen transfer process between 6.0 ps and 11.5 ps. Color codes are the same as in Figure 1. Bond distances are in Å.

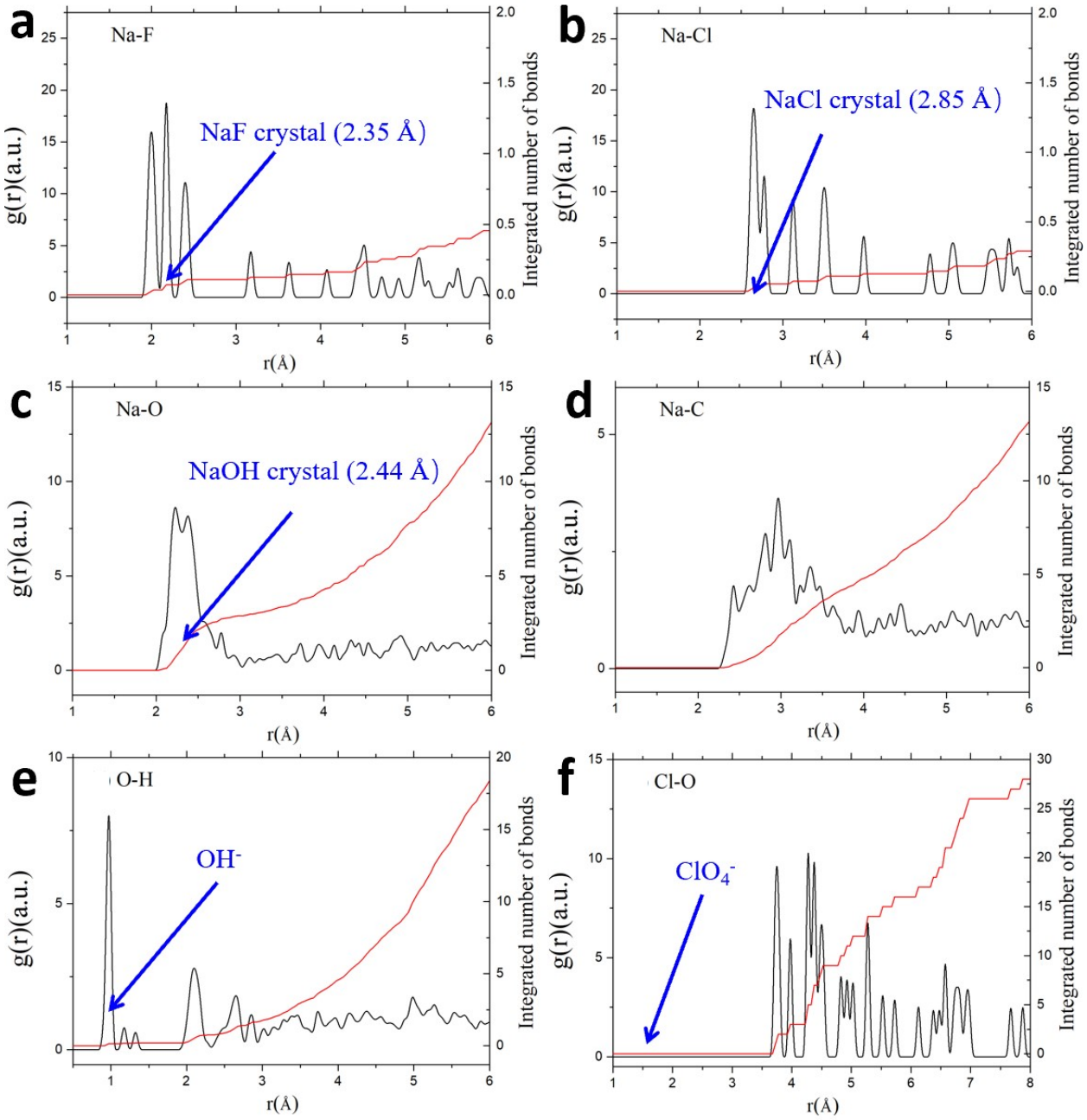

Figure S3. Radial distribution function and integrated number of bonds for (a) Na−F, (b) Na-Cl, (c) Na-O, (d) Na-C, (e) O-H and (f) Cl-O. Red lines and black lines represent the radial distribution function and integrated number of bonds, respectively.

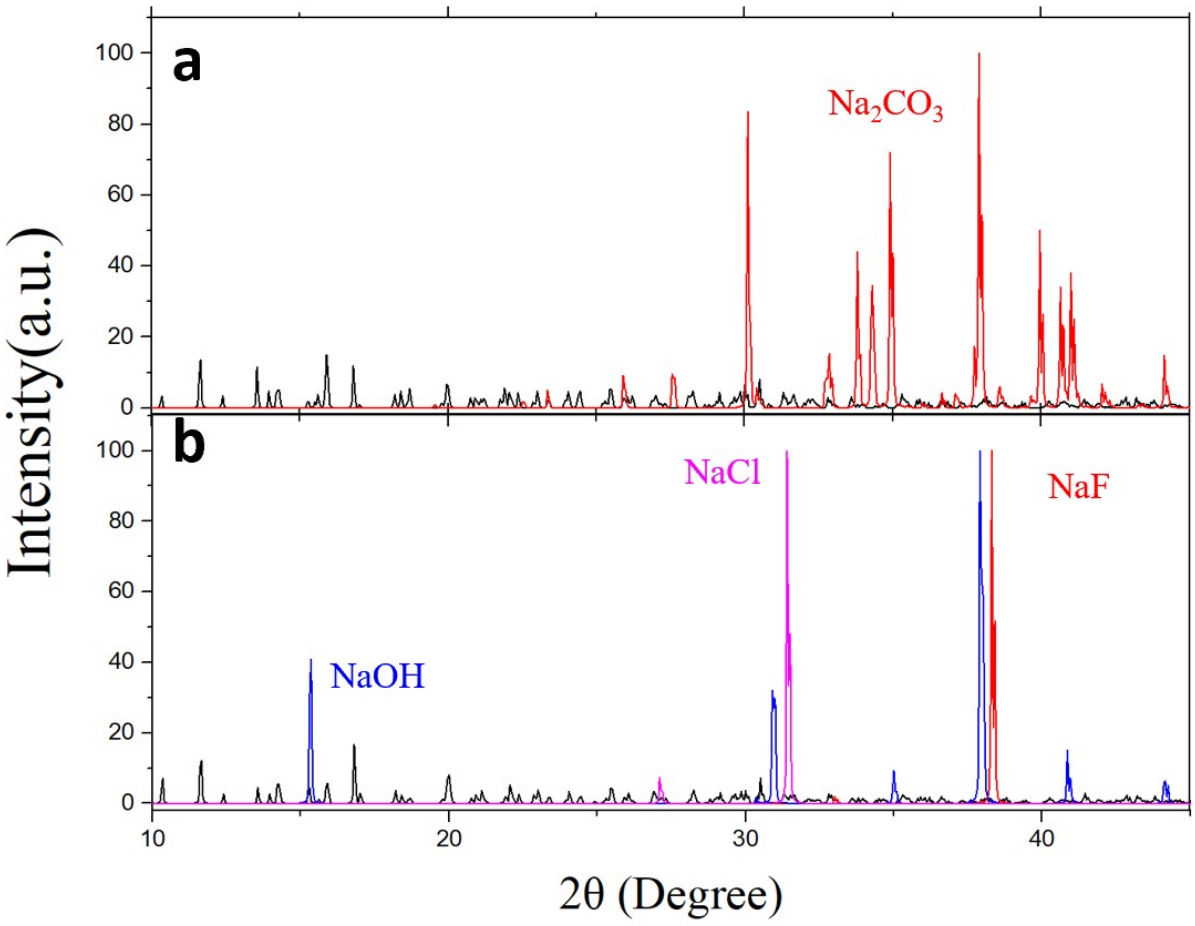

Figure S4. (a) XRD patterns from HAIR MD simulations at 275 ps. (b) XRD patterns from HAIR MD simulations at 2800 ps.

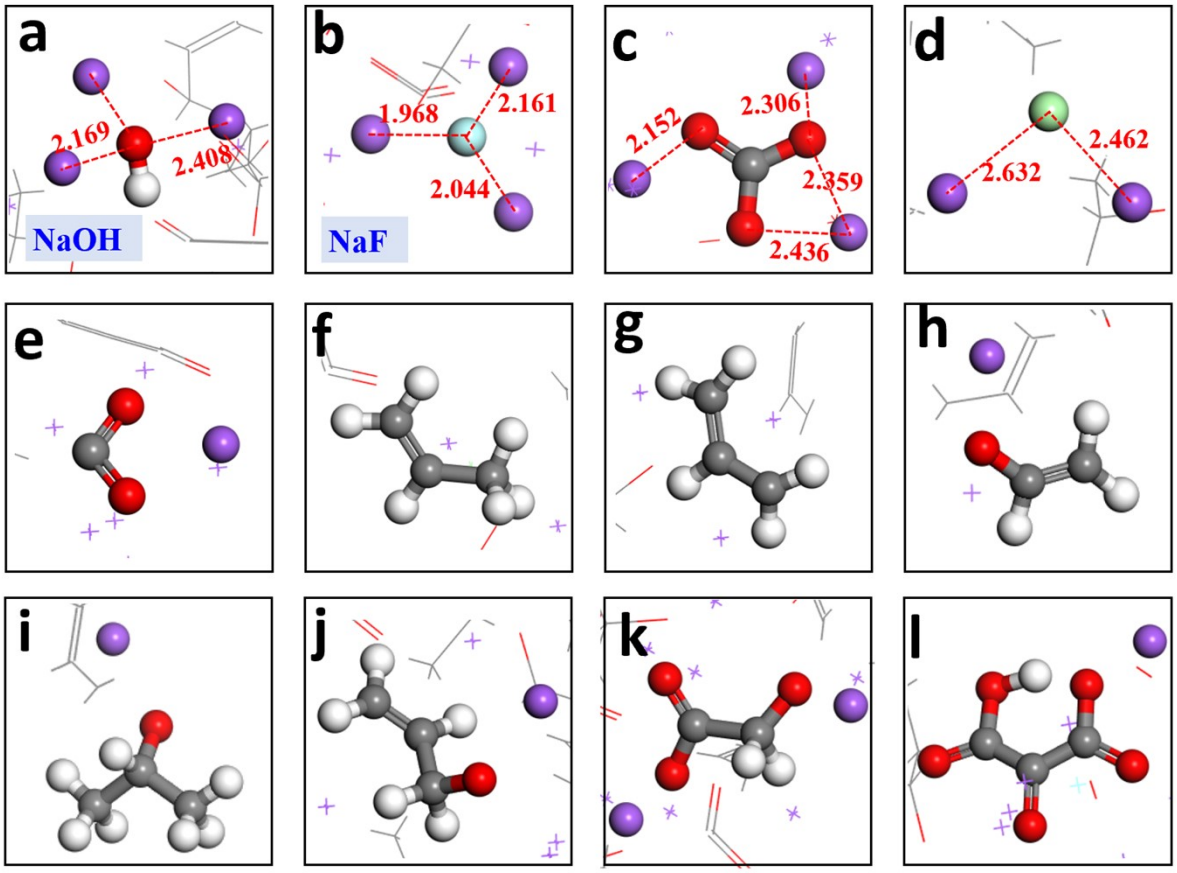

Figure S5. The possible products obtained from HAIR MD simulations. (a) NaOH. (b) NaF. (c) Na_2CO_3. (d) NaCl. (e) CO_2. (f) C_3H_6. (g) C_3H_5. (h) $NaOC_2H_3$. (i) $NaOC_3H_7$. (j) $NaOC_3H_5$. (k) $Na_2O(O)CH_2O$. (h) NOC_3O_3OH.

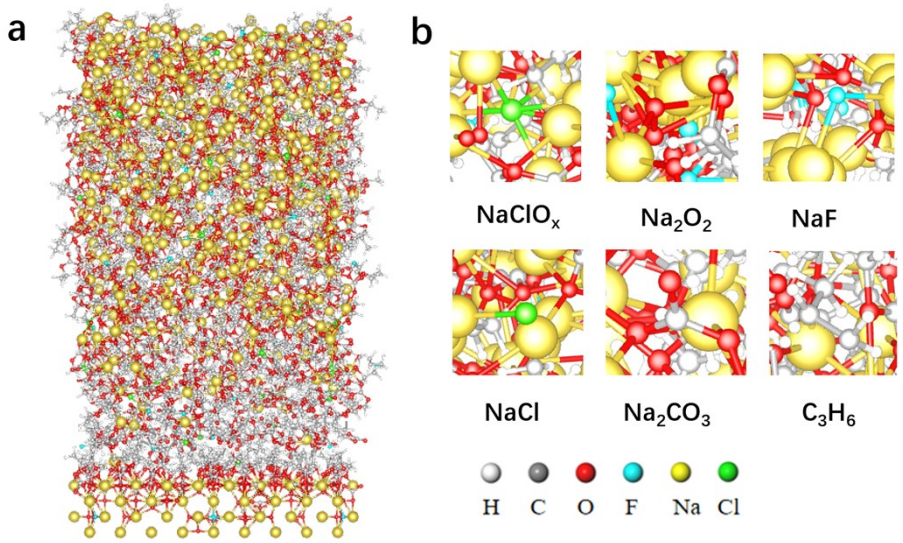

Figure S6. (a) The final snapshot and (b) the atomic structures of major products after 1 ns RMD simulation.

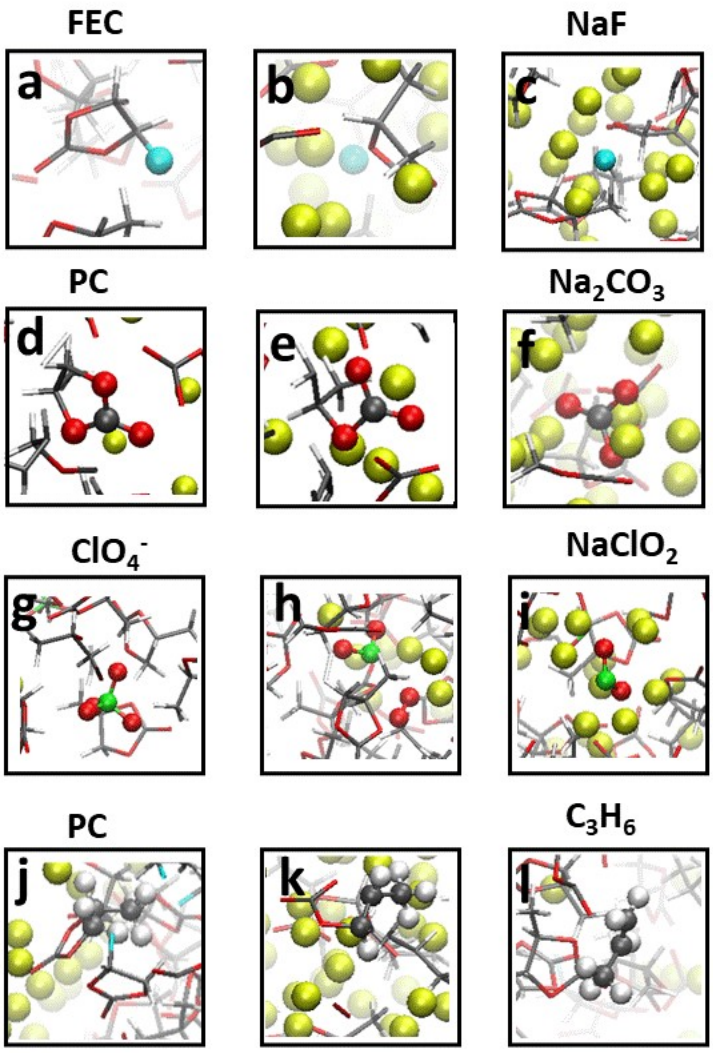

Figure S7. The formation processes of the species in ReaxFF MD simulations. (a-c) The formation of NaF from FEC. (d-f) The formation of Na_2CO_3 from PC. (g-i) The formation of $NaClO_2$ from ClO_4^-. (j-l) The formation of C_3H_6 from PC.

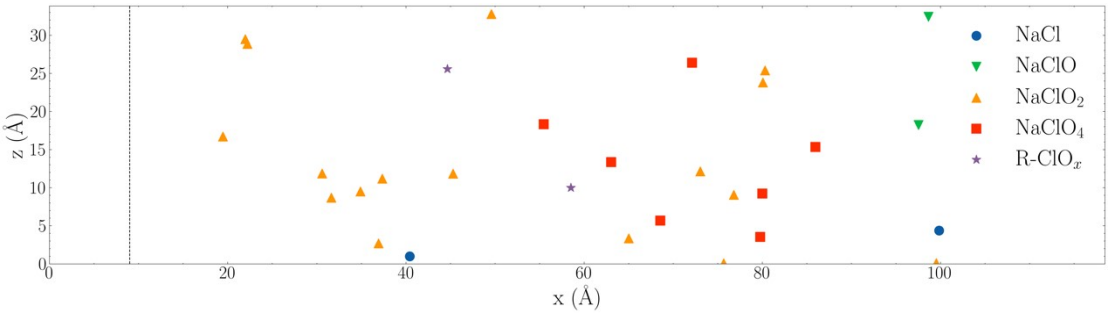

Figure S8. 2D (z-x) spatial distribution of Cl in different compounds (NaCl, NaClO, $NaClO_2$, $NaClO_4$ and R-ClO_x) projected along the y-direction from the 1 ns RMD simulation. The interface at 9 nm between the Na-anode and electrolyte is shown as a black dashed line.

Table S1. The geometries of the training set using the QM and ReaxFF methods.

Molecule	Bond/Angle	QM (B3LYP/6-311+G**)	ReaxFF
$HClO_4$	Cl_1-O_2	1.448	1.512
	Cl_1-O_3	1.460	1.512
	O_2- Cl_1-O_4	115.2	108.5
	O_2- Cl_1-O_5	100.6	110.4
	O_3- Cl_1-O_4	113.6	108.4
$HClO_3$	Cl_1-O_2	1.483	1.515
	Cl_1-O_3	1.483	1.515
	O_2- Cl_1-O_4	115.2	117.7
	O_3- Cl_1-O_5	115.2	117.7
	O_2- Cl_1-O_3	113.4	116.4
$HClO_2$	Cl_1-O_2	1.546	1.508
	O_2- Cl_1-O_3	113.7	116.3

Table S2. The relative reaction energies (in kcal/mol) for QM and ReaxFF calculations.

Reaction	QM (B3LYP/6-311+G**)	ReaxFF
$HClO_4$=$HClO_3$+O(3p)	28.4	36.6
$HClO_3$=$HClO_2$+O(3p)	39.5	38.5
$HClO_2$=HClO+O(3p)	20.9	22.4

Table S3. Calculated binding energy and corresponding values in experiments.

Species (Na 1 s, O 1 s, C1s)	Calculated Binding energy (eV)	Experimental Binding energy (eV)	Calculated Binding energy shift (eV)	Experimental Binding energy shift (eV)
Na-O	1029.6	1027.1	0	0
Na-F	1030.4	1027.7	0.8	0.6
C-*O*-Na	505.3	531.8	0	0
Na*O*H	506.2	532.8	0.9	1
C=*O*	506.7	532.9	1.4	1.1
C=C	264.7	284.3	-0.7	-0.7
C-C/*C*-H	265.4	285	0	0
C-O	266.7	286.3	1.3	1.3
C=O	267.3	287.8	1.9	2.8
O=*C*-O	268.6	288.6	3.2	3.6

Note: The binding energy shift values in Na 1 s, O 1 s and C 1 s are shifted to Na-O, C-O-Na and C-C/C-H, respectively.

Table S4. The number (N) of major products from 1 ns ReaxFF MD simulations of two independent simulations (Samples 1 and 2) starting from different initial configurations.

Mol.	**Na_2CO_3**	**C_3H_5**	**CO_2**	**NaF**	**NaCl**	**NaOH**
No.	1	4	5	2	1	4

Table S5. The number (N) of major products from 1ns ReaxFF MD simulations.

Mol.	**Na_2O_2**	**Na_2CO_3**	**C_3H_6**	**Na_2O**	**$NaClO_2$**	**NaF**	**NaCl**	**NaOH**
No.	27	15	15	17	14	9	4	0

Table S5. The number (N) of major products from 2.8 ns HAIR MD simulations.

Sample	Na_2CO_3	C_3H_5	CO_2	NaF	NaCl	NaOH
1	1	4	5	2	2	4

Table S6. The number (N) of major Cl-containing products from 1 ns RMD simulations.

Mol.	**NaCl**	**NaClO**	**$NaClO_2$**	**$NaClO_4$**	**R-ClO_x**
No.	2	2	17	7	2

Appendix: Force field parameters.

```
39       ! Number of general parameters
  50.0000 !p_boc1 Eq(4c): Overcoordination parameter
   9.5469 !p_boc2 Eq(4d): Overcoordination parameter
  26.5405 !p_coa2 Eq(15): Valency angle conjugation
   1.7224 !p_trip4 Eq(20): Triple bond stabilisation
   6.8702 !p_trip3 Eq(20): Triple bond stabilisation
  60.4850 !k_c2 Eq(19): C2-correction
   1.0588 !p_ovun6 Eq(12): Undercoordination
   4.6000 !p_trip2 Eq(20): Triple bond stabilisation
  12.1176 !p_ovun7 Eq(12): Undercoordination
  13.3056 !p_ovun8 Eq(12): Undercoordination
 -70.5044 !p_trip1 Eq(20): Triple bond stabilization
   0.0000 !Lower Taper-radius (must be 0)
  10.0000 !R_cut Eq(21): Upper Taper-radius
   2.8793 !p_fe1 Eq(6a): Fe dimer correction
  33.8667 !p_val6 Eq(13c): Valency undercoordination
   6.0891 !p_lp1 Eq(8): Lone pair param
   1.0563 !p_val9 Eq(13f): Valency angle exponent
   2.0384 !p_val10 Eq(13g): Valency angle parameter
   6.1431 !p_fe2 Eq(6a): Fe dimer correction
   6.9290 !p_pen2 Eq(14a): Double bond/angle param
   0.3989 !p_pen3 Eq(14a): Double bond/angle param
   3.9954 !p_pen4 Eq(14a): Double bond/angle param
  -2.4837 !p_fe3 Eq(6a): Fe dimer correction
   5.7796 !p_tor2 Eq(16b): Torsion/BO parameter
  10.0000 !p_tor3 Eq(16c): Torsion overcoordination
```

1.9487 !p_tor4 Eq(16c): Torsion overcoordination

-1.2327 !p_elho Eq(26a): electron-hole interaction

2.1645 !p_cot2 Eq(17b): Conjugation if tors13=0

1.5591 !p_vdW1 Eq(23b): vdWaals shielding

0.1000 !Cutoff for bond order (*100)

2.1365 !p_coa4 Eq(15): Valency angle conjugation

0.6991 !p_ovun4 Eq(11b): Over/Undercoordination

50.0000 !p_ovun3 Eq(11b): Over/Undercoordination

1.8512 !p_val8 Eq(13d): Valency/lone pair param

0.5000 !X_soft Eq(25): ACKS2 softness for X_ij

20.0000 !d Eq(23d): Scale factor in lg-dispersion

5.0000 !p_val Eq(27): Gauss exponent for electrons

0.0000 !1 Eq(13e): disable undecoord in val angle

2.6962 !p_coa3 Eq(15): Valency angle conjugation

11 ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
cov r3;Elp;Heat inc.;bo131;bo132;bo133;softcut;n.u.
ov/un;val1;n.u.;val3,vval4

C 1.3817 4.0000 12.0000 1.8903 0.1838 0.9000 1.1341 4.0000
9.7559 2.1346 4.0000 34.9350 79.5548 5.9666 7.0000 0.0000
1.2114 0.0000 202.5551 8.9539 34.9289 13.5366 0.8563 0.0000
-2.8983 2.5000 1.0564 4.0000 2.9663 0.0000 0.0000 0.0000

H 0.8930 1.0000 1.0080 1.3550 0.0930 0.8203 -0.1000 1.0000
8.2230 33.2894 1.0000 0.0000 121.1250 3.7248 9.6093 1.0000
-0.1000 0.0000 61.6606 3.0408 2.4197 0.0003 1.0698 0.0000
-19.4571 4.2733 1.0338 1.0000 2.8793 0.0000 0.0000 0.0000

O 1.2450 2.0000 15.9990 2.3890 0.1000 1.0898 1.0548 6.0000

9.7300 13.8449 4.0000 37.5000 116.0768 8.5000 8.3122 2.0000

0.9049 0.4056 59.0626 3.5027 0.7640 0.0021 0.9745 0.0000

-3.5500 2.9000 1.0493 4.0000 2.9225 0.0000 0.0000 0.0000

Cs 0.0100 1.0000 132.9054 2.6059 0.3922 0.5510 -1.0000 1.0000

9.0000 2.5000 1.0000 0.0000 0.0000 -3.1185 6.7714 0.0000

-1.0000 0.0000 23.0445 100.0000 1.0000 0.0000 0.8563 0.0000

-2.5000 3.9900 1.0338 8.0000 2.5791 1.0000 0.0100 13.0000

K 0.0100 1.0000 39.0983 2.1226 0.1000 0.4000 -1.0000 1.0000

9.0027 2.5000 1.0000 0.0000 0.0000 -2.8800 7.1848 0.0000

-1.0000 0.0000 23.0445 100.0000 1.0000 0.0000 0.8563 0.0000

-2.5000 3.9900 1.0338 8.0000 2.5791 1.0000 0.0100 13.0000

Na 0.0001 1.0000 22.9898 2.6441 0.2588 0.8011 -1.0000 1.0000

9.0003 2.5000 1.0000 0.0000 0.0000 -3.4731 8.6438 0.0000

-1.0000 0.0000 23.0445 100.0000 1.0000 0.0000 0.8563 0.0000

-4.1479 3.9900 1.0338 8.0000 2.5791 0.0000 0.0000 0.0000

Cl 1.5046 1.0000 35.4500 3.0207 0.0568 0.3640 -1.0000 7.0000

10.5008 10.1330 1.0000 0.0000 0.0000 10.0000 6.0403 2.0000

-1.0000 0.0100 35.1770 6.2293 5.2294 0.1542 0.8563 0.0000

-10.2080 2.9867 1.0338 6.2998 2.5791 0.0000 0.0000 0.0000

I 1.9000 1.0000 126.9000 3.1000 0.1500 0.8298 -1.0000 7.0000

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-1.0000 2.3407 35.1770 6.2293 5.2294 0.1542 0.8563 0.0000

-10.2080 2.9867 1.0338 6.2998 2.5791 0.0000 0.0000 0.0000

F 1.1846 1.0000 18.9984 1.7922 0.1267 0.4038 -0.1000 7.0000

10.3184 7.5000 1.0000 9.2533 0.2000 9.3891 6.5612 2.0000

-1.0000 3.5571 18.0000 6.9821 4.1799 1.0561 0.0000 0.0000

-7.3000 2.6656 1.0493 4.0000 2.9225 0.0000 0.0000 0.0000

```
Li   0.0001   1.0000   6.9410   2.6000   0.0865   0.8380  -0.1000   1.0000
     9.6984   1.4649   1.0000   0.0000   0.0000  -4.0561   9.7698   0.0000
    -1.0000   0.0000  37.5000   5.4409   6.9107   0.1973   0.8563   0.0000
   -24.7916   2.2989   1.0338   1.0000   2.8103   1.3000   0.2000  13.0000
X   -0.1000   2.0000   1.0080   2.0000   0.0000   1.0000  -0.1000   6.0000
    10.0000   2.5000   4.0000   0.0000   0.0000   8.5000   1.5000   0.0000
    -0.1000   0.0000 127.6226   8.7410  13.3640   0.6690   0.9745   0.0000
   -11.0000   2.7466   1.0338   6.2998   2.8793   0.0000   0.0000   0.0000
42    ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                      pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr
 1  1 158.2004  99.1897  78.0000  -0.7738  -0.4550   1.0000  37.6117   0.4147
       0.4590  -0.1000   9.1628   1.0000  -0.0777   6.7268   1.0000   0.0000
 1  2 169.4760   0.0000   0.0000  -0.6083   0.0000   1.0000   6.0000   0.7652
       5.2290   1.0000   0.0000   1.0000  -0.0500   6.9136   0.0000   0.0000
 2  2 153.3934   0.0000   0.0000  -0.4600   0.0000   1.0000   6.0000   0.7300
       6.2500   1.0000   0.0000   1.0000  -0.0790   6.0552   0.0000   0.0000
 1  3 158.6946 107.4583  23.3136  -0.4240  -0.1743   1.0000  10.8209   1.0000
       0.5322  -0.3113   7.0000   1.0000  -0.1447   5.2450   0.0000   0.0000
 3  3 142.2858 145.0000  50.8293   0.2506  -0.1000   1.0000  29.7503   0.6051
       0.3451  -0.1055   9.0000   1.0000  -0.1225   5.5000   1.0000   0.0000
 2  3 160.0000   0.0000   0.0000  -0.5725   0.0000   1.0000   6.0000   0.5626
       1.1150   1.0000   0.0000   1.0000  -0.0920   4.2790   0.0000   0.0000
 2  4   0.0000   0.0000   0.0000  -1.0000  -0.3000   1.0000  36.0000   0.7000
      10.1151  -0.3500  25.0000   1.0000  -0.1053   8.2003   1.0000   0.0000
 3  4   9.8700   0.0000  43.0000  -0.3792  -0.3000   1.0000  36.0000   0.1000
       6.7692  -0.3500  25.0000   1.0000  -0.0656   7.1227   1.0000   0.0000
 4  4  17.6609   0.0000   0.0000   0.5700   0.3000   0.0000  25.0000   0.6157
```

0.4946 -0.4000 12.0000 1.0000 -0.0557 4.5153 0.0000 0.0000

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10.1151 -0.3500 25.0000 1.0000 -0.1053 8.2003 1.0000 0.0000

3 5 22.6146 0.0000 43.0000 0.6651 -0.3000 1.0000 36.0000 1.0000

0.9166 -0.3500 25.0000 1.0000 -0.0583 7.3861 1.0000 0.0000

5 5 22.6628 0.0000 0.0000 0.3272 0.3000 0.0000 25.0000 0.5944

0.9915 -0.4000 12.0000 1.0000 -0.0517 4.5075 0.0000 0.0000

4 5 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

2 6 26.7569 0.0000 0.0000 1.0000 -0.3000 1.0000 36.0000 0.0100

0.5785 -0.3500 25.0000 1.0000 -0.2601 6.6137 1.0000 0.0000

3 6 27.9718 0.0000 0.0000 0.0437 -0.3000 1.0000 36.0000 0.0100

19.6220 -0.3500 25.0000 1.0000 -0.1279 7.3318 1.0000 0.0000

6 6 0.0000 0.0000 0.0000 -0.7273 0.3000 0.0000 25.0000 0.1919

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2 7 150.6697 0.0000 0.0000 -0.6499 -0.2000 0.0000 16.0000 0.8645

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3 7 182.6922 0.0000 0.0000 -0.0609 -0.2230 0.8849 48.3524 -0.1313

20.2009 -0.5687 16.1402 0.8691 -0.2518 5.8334 0.1025 0.3896

7 7 148.6765 0.0000 0.0000 0.7040 -0.3500 0.0000 25.0000 0.9428

-0.3546 -0.2500 15.0000 1.0000 -0.1329 7.0417 0.0000 0.0000

2 8 119.4286 0.0000 0.0000 -1.0000 -0.2000 0.0000 16.0000 0.6889

0.8475 -0.2000 15.0000 1.0000 -0.1744 7.4576 0.0000 0.0000

3 8 0.0000 0.0000 0.0000 0.5000 -0.2000 0.0000 16.0000 0.5000

1.0001 -0.2000 15.0000 1.0000 -0.1000 15.0000 0.0000 0.0000

8 8 148.6765 0.0000 0.0000 0.7040 -0.3500 0.0000 25.0000 0.9428

-0.3546 -0.2500 15.0000 1.0000 -0.1329 7.0417 0.0000 0.0000

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16.3699 -0.2000 15.0000 1.0000 -0.2265 7.1308 0.0000 0.0000

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0.0992 -0.2000 15.0000 1.0000 -0.0687 5.9021 0.0000 0.0000

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0.3634 -0.2000 15.0000 1.0000 -0.0509 6.6722 0.0000 0.0000

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5 8 12.3160 0.0000 0.0000 -0.1822 -0.2000 0.0000 16.0000 0.2459

0.6720 -0.2000 15.0000 1.0000 -0.0500 6.3614 0.0000 0.0000

4 7 8.6575 0.0000 0.0000 -0.1496 -0.2000 0.0000 16.0000 0.6476

0.1466 -0.2000 15.0000 1.0000 -0.1292 4.7220 0.0000 0.0000

1 4 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

1 5 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

1 6 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

1 7 0.0000 0.0000 0.0000 0.5000 -0.3000 1.0000 16.0000 0.5000

0.5000 -0.2500 15.0000 1.0000 -0.1000 9.0000 0.0000 0.0000

6 9 30.0000 0.0000 0.0000 0.9241 -0.2000 0.0000 16.0000 0.2072

0.3634 -0.2000 15.0000 1.0000 -0.0509 6.6722 0.0000 0.0000

1 9 185.5818 0.0000 0.0000 -0.6890 -0.5000 1.0000 35.0000 0.9001

```
      4.7476  -0.2500  15.0000   1.0000  -0.1113   4.1292   1.0000   0.0000
 5  7  28.7935   0.0000   0.0000  -0.8610  -0.2000   0.0000  16.0000   0.1362
      6.3616  -0.2000  15.0000   1.0000  -0.0477   5.8987   0.0000   0.0000
 6  7   9.0644   0.0000   0.0000  -0.9774  -0.3000   1.0000  16.0000   0.5363
      1.3533  -0.2500  15.0000   1.0000  -0.0340   5.1590   0.0000   0.0000
 2 10   0.0000   0.0000   0.0000   1.0000  -0.3000   1.0000  36.0000   0.0100
      0.3415  -0.3500  25.0000   1.0000  -0.2770   6.4396   1.0000   0.0000
 3 10  71.3512  -0.0200   0.0000   0.6715   0.3000   0.0000   6.0000   0.1621
      0.1284  -0.2500  11.9965   1.0000  -0.1026   5.8179   0.0000   0.0000
 7 10  39.6304   0.0000   0.0000  -0.6878  -0.3000   1.0000  16.0000   0.4891
      1.8957  -0.2500  15.0000   1.0000  -0.0471   5.0000   0.0000   0.0000
10 10   0.0000   0.0000   0.0000   0.3228   0.3000   0.0000  26.0000   0.6003
      1.7161   0.0000  12.0000   1.0000  -0.1015   4.0000   0.0000   0.0000
31    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
 1  2   0.1239   1.4004   9.8467   1.1210  -1.0000  -1.0000
 2  3   0.0283   1.2885  10.9190   0.9215  -1.0000  -1.0000
 1  3   0.1156   1.8520   9.8317   1.2854   1.1352   1.0706
 2  4   0.3000   1.6894  14.0000  -1.0000  -1.0000  -1.0000
 3  4   0.1997   1.7894  12.7397   1.8422  -1.0000  -1.0000
 2  5   0.3000   1.5647  13.3924  -1.0000  -1.0000  -1.0000
 3  5   0.1832   1.7503  12.6152   1.6986  -1.0000  -1.0000
 2  6   0.1100   1.8410   9.1430   1.7735  -1.0000  -1.0000
 3  6   0.1536   1.6000  12.9050   1.6436  -1.0000  -1.0000
 2  7   0.1695   1.6156   9.7834   1.4740  -1.0000  -1.0000
 3  7   0.1164   2.2898   9.9235  -0.5309  -1.0000  -1.0000
 2  8   0.2500   1.9082   9.7544   1.6395  -1.0000  -1.0000
 3  8   0.0879   2.1404  10.1167  -1.0000  -1.0000  -1.0000
```

2 9 0.0553 1.7443 9.0006 1.3514 -1.0000 -1.0000

3 9 0.1547 2.1287 9.6188 -1.0000 -1.0000 -1.0000

4 9 0.2002 2.1104 11.4482 1.9513 -1.0000 -1.0000

5 9 0.1775 1.9529 10.3353 1.6962 -1.0000 -1.0000

4 8 0.4745 2.4978 12.1514 2.1186 -1.0000 -1.0000

5 8 0.2726 2.3895 11.6451 2.1295 -1.0000 -1.0000

4 7 0.2710 2.1676 12.2929 1.9891 -1.0000 -1.0000

1 4 0.2000 1.8500 11.0000 -1.0000 -1.0000 -1.0000

1 5 0.2000 1.8500 11.0000 -1.0000 -1.0000 -1.0000

1 6 0.2000 1.8500 11.0000 -1.0000 -1.0000 -1.0000

1 7 0.2000 1.8500 11.0000 -1.0000 -1.0000 -1.0000

1 8 0.2000 1.8500 11.0000 -1.0000 -1.0000 -1.0000

1 9 0.0501 1.6854 11.0421 1.2644 -1.0000 -1.0000

6 7 0.2193 1.8308 12.0561 1.7244 -1.0000 -1.0000

5 7 0.2264 2.0209 12.8644 2.2260 -1.0000 -1.0000

2 10 0.5000 1.4607 13.0000 -1.0000 -1.0000 -1.0000

3 10 0.0696 1.8520 10.0874 1.5559 -1.0000 1.0000

7 10 0.2331 1.6173 12.1979 1.7675 -1.0000 -1.0000

65 ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2

1 1 1 59.0573 30.7029 0.7606 0.0000 0.7180 6.2933 1.1244

1 1 2 65.7758 14.5234 6.2481 0.0000 0.5665 0.0000 1.6255

2 1 2 70.2607 25.2202 3.7312 0.0000 0.0050 0.0000 2.7500

1 2 2 0.0000 0.0000 6.0000 0.0000 0.0000 0.0000 1.0400

1 2 1 0.0000 3.4110 7.7350 0.0000 0.0000 0.0000 1.0400

2 2 2 0.0000 27.9213 5.8635 0.0000 0.0000 0.0000 1.0400

1 1 3 67.7237 22.2598 1.6663 0.0000 2.0753 0.0000 1.2458

3 1 3 99.7513 33.0725 1.8107 -13.5356 1.3482 -46.1315 1.8413

2 1 3 65.0000 13.8815 5.0583 0.0000 0.4985 0.0000 1.4900

1 3 1 73.5312 44.7275 0.7354 0.0000 3.0000 0.0000 1.0684

1 3 3 79.4761 36.3701 1.8943 0.0000 0.7351 67.6777 3.0000

3 3 3 80.7324 30.4554 0.9953 0.0000 1.6310 50.0000 1.0783

1 3 2 70.1880 20.9562 0.3864 0.0000 0.0050 0.0000 1.6924

2 3 3 75.6935 50.0000 2.0000 0.0000 1.0000 0.0000 1.1680

2 3 2 85.8000 9.8453 2.2720 0.0000 2.8635 0.0000 1.5800

1 2 3 0.0000 25.0000 3.0000 0.0000 1.0000 0.0000 1.0400

3 2 3 0.0000 15.0000 2.8900 0.0000 0.0000 0.0000 2.8774

2 2 3 0.0000 8.5744 3.0000 0.0000 0.0000 0.0000 1.0421

3 4 3 99.7500 0.5445 8.0762 0.0000 4.0000 0.0000 1.3928

2 3 4 99.3112 3.0043 9.4051 0.0000 3.7889 0.0000 1.1216

4 3 4 97.3143 0.1000 0.2763 0.0000 3.5792 0.0000 3.9750

3 5 3 100.0000 1.2360 6.8249 0.0000 3.2930 0.0000 1.0000

2 3 5 100.0000 1.0007 9.7740 0.0000 1.4276 0.0000 1.0000

5 3 5 98.5744 2.1499 1.6268 0.0000 3.7347 0.0000 2.8271

3 2 7 0.0000 0.5102 0.0100 0.0000 0.0000 0.0000 1.3399

7 2 7 0.0000 5.0000 1.0000 0.0000 1.0000 0.0000 1.2500

3 7 3 71.0495 23.9532 5.9373 -9.0127 -0.2745 -0.6384 2.2117

3 2 8 0.0000 1.4821 5.0000 0.0000 0.0000 0.0000 2.9750

3 2 9 0.0000 1.8088 0.0100 0.0000 0.0000 0.0000 1.2229

2 9 2 0.0000 6.9640 1.4314 0.0000 0.0000 0.0000 1.0400

4 9 4 0.0000 2.0000 1.0000 0.0000 1.0000 0.0000 1.0000

9 4 9 40.0000 1.0000 1.0000 0.0000 1.0000 0.0000 1.0000

4 9 9 0.0000 10.0000 1.0000 0.0000 1.0000 0.0000 1.4000

4 4 9 20.0000 0.0000 1.0000 0.0000 1.0000 0.0000 1.4000

5 9 5 0.0000 0.5000 1.0000 0.0000 1.0000 0.0000 1.2000

9 5 9 40.0000 0.5000 1.0000 0.0000 1.0000 0.0000 1.2000

5 9 9 0.0000 10.0000 1.0000 0.0000 1.0000 0.0000 1.4000

4 8 4 0.0000 2.0000 1.0000 0.0000 1.0000 0.0000 1.0000

8 4 8 40.0000 1.0000 1.0000 0.0000 1.0000 0.0000 1.0000

4 8 8 0.0000 10.0000 1.0000 0.0000 1.0000 0.0000 1.4000

4 4 8 20.0000 0.0000 1.0000 0.0000 1.0000 0.0000 1.4000

5 8 5 0.0000 0.5000 1.0000 0.0000 1.0000 0.0000 1.2000

8 5 8 40.0000 0.5000 1.0000 0.0000 1.0000 0.0000 1.2000

5 8 8 0.0000 10.0000 1.0000 0.0000 1.0000 0.0000 1.4000

4 7 4 0.0000 0.5000 1.0000 0.0000 1.0000 0.0000 1.0000

7 4 7 40.0000 1.0000 1.0000 0.0000 1.0000 0.0000 1.0000

4 7 7 0.0000 10.0000 1.0000 0.0000 1.0000 0.0000 1.4000

4 4 7 20.0000 0.0000 1.0000 0.0000 1.0000 0.0000 1.4000

5 7 5 0.0000 0.5000 1.0000 0.0000 1.0000 0.0000 1.2000

7 5 7 40.0000 0.5000 1.0000 0.0000 1.0000 0.0000 1.2000

1 1 9 75.1647 40.0000 7.6174 0.0000 2.9750 0.0000 3.2465

9 1 9 76.5153 40.0000 6.1232 0.0000 3.0000 0.0000 1.0000

2 1 9 85.4658 0.0100 1.9807 0.0000 1.4400 0.0000 2.9068

3 1 9 70.0000 35.0000 2.0000 0.0000 1.0000 0.0000 1.2500

3 5 8 0.0000 3.0602 2.0000 0.0000 0.5000 0.0000 1.0000

3 4 9 0.0000 8.0000 2.0000 0.0000 0.5000 0.0000 1.0000

3 5 9 0.0000 3.7500 2.0000 0.0000 0.5000 0.0000 1.0000

3 6 3 100.0000 40.0000 7.8728 0.0000 3.2930 0.0000 2.6836

2 3 6 82.0800 5.5605 8.0000 0.0000 1.4276 0.0000 1.6766

6 3 6 81.0000 4.7500 0.9000 0.0000 1.0000 0.0000 2.0000

3 10 3 1.0000 6.7901 5.5000 0.0000 0.2366 0.0000 1.5936

2 3 10 100.0000 4.9629 8.0000 0.0000 0.1000 0.0000 1.0000

10 3 10 100.0000 8.0985 3.1295 0.0000 2.0000 0.0000 1.1755

3 10 7 54.0553 22.2701 8.0000 0.0000 2.3740 0.0000 2.0553

2 7 10 92.8098 7.7675 0.2250 0.0000 0.5870 0.0000 3.0000

30 ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n

1 1 1 1 -0.2500 34.7453 0.0288 -6.3507 -1.6000 0.0000 0.0000

1 1 1 2 -0.2500 29.2131 0.2945 -4.9581 -2.1802 0.0000 0.0000

2 1 1 2 -0.2500 31.2081 0.4539 -4.8923 -2.2677 0.0000 0.0000

1 1 1 3 -0.3495 22.2142 -0.2959 -2.5000 -1.9066 0.0000 0.0000

2 1 1 3 0.0646 24.3195 0.6259 -3.9603 -1.0000 0.0000 0.0000

3 1 1 3 -0.5456 5.5756 0.8433 -5.1924 -1.0180 0.0000 0.0000

1 1 3 1 1.7555 27.9267 0.0072 -2.6533 -1.0000 0.0000 0.0000

1 1 3 2 -1.4358 36.7830 -1.0000 -8.1821 -1.0000 0.0000 0.0000

2 1 3 1 -1.3959 34.5053 0.7200 -2.5714 -2.1641 0.0000 0.0000

2 1 3 2 -2.5000 70.0597 1.0000 -3.5539 -2.9929 0.0000 0.0000

1 1 3 3 0.6852 11.2819 -0.4784 -2.5000 -2.1085 0.0000 0.0000

2 1 3 3 0.1933 80.0000 1.0000 -4.0590 -3.0000 0.0000 0.0000

3 1 3 1 -1.9889 76.4820 -0.1796 -3.8301 -3.0000 0.0000 0.0000

3 1 3 2 0.2160 72.7707 -0.7087 -4.2100 -3.0000 0.0000 0.0000

3 1 3 3 -2.5000 71.0772 0.2542 -3.1631 -3.0000 0.0000 0.0000

1 3 3 1 2.5000 -0.6002 1.0000 -3.4297 -2.8858 0.0000 0.0000

1 3 3 2 -2.5000 -3.3822 0.7004 -5.4467 -2.9586 0.0000 0.0000

2 3 3 2 2.5000 -4.0000 0.9000 -2.5000 -1.0000 0.0000 0.0000

1 3 3 3 1.2329 -4.0000 1.0000 -2.5000 -1.7479 0.0000 0.0000

2 3 3 3 0.8302 -4.0000 -0.7763 -2.5000 -1.0000 0.0000 0.0000

3 3 3 3 -2.5000 -4.0000 1.0000 -2.5000 -1.0000 0.0000 0.0000

0 1 2 0 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

0 2 2 0 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

0 2 3 0 0.0000 0.1000 0.0200 -2.5415 0.0000 0.0000 0.0000

0 1 1 0 0.0000 50.0000 0.3000 -4.0000 -2.0000 0.0000 0.0000

0 3 3 0 0.5511 25.4150 1.1330 -5.1903 -1.0000 0.0000 0.0000

1 1 3 3 -2.0000 73.0530 1.5000 -9.0000 -2.0000 0.0000 0.0000

1 3 3 1 0.0002 80.0000 -1.5000 -2.5000 -2.0000 0.0000 0.0000

3 1 3 3 -1.8835 20.0000 1.5000 -9.0000 -2.0000 0.0000 0.0000

2 3 10 3 0.0918 64.5743 -1.0000 -4.4228 0.0000 0.0000 0.0000

7 ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1

3 2 3 2.1200 -3.5800 1.4500 19.5000

3 2 7 1.8833 -3.6250 1.4500 19.5000

7 2 3 1.8487 -0.0100 1.4500 19.5000

3 2 8 2.4000 -3.9750 1.4500 19.5000

8 2 3 2.2086 -3.9633 1.4500 19.5000

3 2 9 1.5033 -0.0100 1.4500 19.5000

9 2 3 1.7547 -0.2589 1.4500 19.5000